Exploring Modern Technologies for NMR Processing Software

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NMR data is different from other forms of analytical data, in that datasets can be large and contain useful information throughout the measured FIDs. This is primarily due to the nature of the NMR signal, which needs to be Fourier Transformed to become presentable. Moreover, some signal averaging, noise reduction and digital signal processing (DSP) is already performed on the instrument. Therefore, the data compression techniques that could be used in other data types are not applicable to NMR, as they will remove parts of the signal.

Modern software Architecture

There are two main architectures in modern software design: The single-user i.e., the desktop approach and the multi-user server-client web approach.

Single User – Desktop Application

The single-user desktop approach is the traditional way. The application consists of several parts (modules) and requires a powerful computer in order to perform the processing required for NMR. It is single user by default and a multi-user implementation in essence requires multiple installations of the same "heavy" software on many computers.

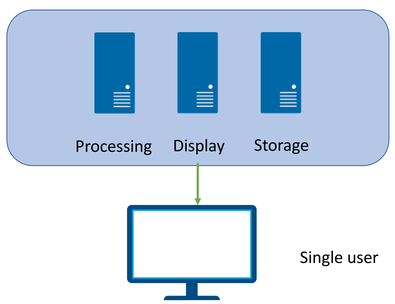

Figure 1. Single user block diagram

Multi-User Server-Client Web

Recently, the server-client web-based, multi-user approach has become more and more popular, specially in larger deployments as these applications are less costly in the long run compared to managing traditional software applications. In this module, various computation-intensive processing tasks are divided amongst several servers and the client computers run a lightweight browser application used only for the lighter display tasks.

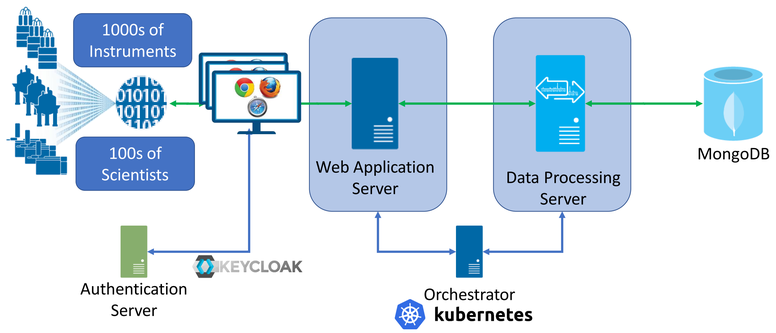

Figure 2. An example for the server-client block diagram

This approach is specifically appealing for NMR data analysis, since only a few high-performance processing computers-server are required. These servers do not necessarily need to be on-premise (cloud implementation). The client computers can be of much lower processing capacity and consequently more economical and accessible. However, there's challenges associated with the transfer of large datasets and the responsiveness of the system, especially in bandwidth-limited environments.

The Next Level of Data Analysis Software

With the constant increase of data size and the recent demands for remote working, scientists need access to convenient processing and analysis tools, while avoiding the hassle that comes with deploying many separate, thick clients (installation, activation, maintenance).
Spectrus JS (JavaScript) is a server-client application that allows facile access to NMR processing and analysis tools for anyone with access to web browser and internet connection. Specific care has been taken for bandwidth-limited connections and system responsiveness. This type of application has been missing from the software portfolio and can bring many advantages to the modern laboratory.

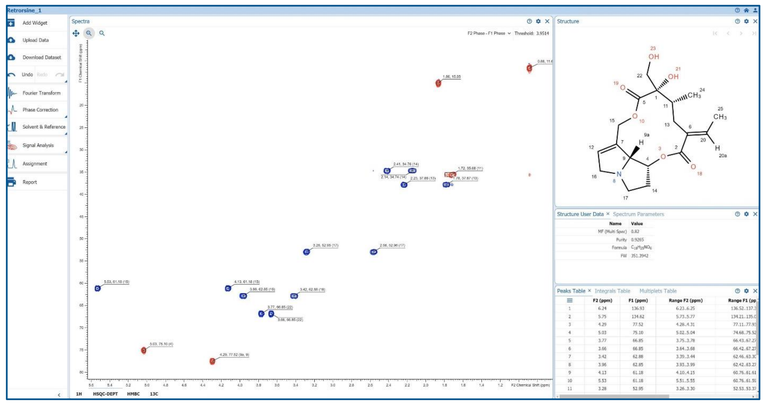

*Figure 3.*A screenshot of the new browser-based, intuitive NMR data analysis application by ACD/Labs

The multi-user, server-client web approach provides advantages for bigger organizations, including easier deployment for many users and reduced hardware requirements and is becoming more popular.